reconstituted as near-native membrane proteins within artificial bilayer systems could be utilized in formulating bioactive surfaces for powerful biomedical and biosensor applications. Novel techniques for re-forming the full-length IMP construct will be discussed.

3190-Pos Board B620
Characterization of Peptides Designed to Control Crystal Nucleation and Growth
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Organisms, from algae to humans are known to mold complex, hierarchical hard tissues from minerals using biomolecular templates and additives. Molecular-level mechanistic understanding of how these biomolecules, particularly proteins, participate in the nucleation and growth of these inorganic crystals has been a longstanding goal. We design peptides with transformative abilities over calcite crystals using Rosetta. Based on the theory of how additives alter crystal nucleation and growth, we employ four modification strategies to modify the morphology of the crystal, viz. a peptide binding to a face, an array of peptides binding to a face, peptides pinning steps and peptides blocking kinks. To test the designs, we employ a variety of techniques ranging from measurements at the atomic scale to full crystal observations. We also investigate alternative mechanisms of modification by comparing the interactions predicted by Rosetta in other select states to those in the target state. For each design, we obtain the solution-state structure of the peptide by circular dichroism. To test peptides designed against a non-native face of calcite, we artificially stabilize the face for binding measurements. The overall crystal morphology change is then tested by incubating supersaturated precursor solutions with the design peptides. To confirm the predicted mechanism of growth alternation, we observe the change in kinetics of calcite step growth with peptide doping using in situ AFM, and report calcite step velocities. Finally, by nucleating calcite on a monolayer of the designed peptides, we examine the face on which calcite nucleated and compare it to our target face. These experimental results provide a feedback loop to the next generation of designs and enable the rational design of bio-surface interactions.

3191-Pos Board B621
Examining Bacterial Cell Interactions using Atomic Force Microscopy
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Given the prevalence of bacterial biofilms in both native and engineered environments, our understanding of their interactions with both other bacteria and abiotic surfaces is quite limited. In this research we use an AFM to analyze the interactions of bacteria such as *E. coli* and a saprophytic, biofilm forming variant of *B. bacteriovorus* with other bacteria and chemically characterized surfaces. Tipless AFM cantilevers were left unmodified (Si3N4), or coated with a monolayer of *E. coli*. These cantilevers were then used to collect force curves on biofilms of *B. bacteriovorus* and *E.coli* as well as chemically characterized surfaces such as mica, silicon, and poly-L-lysine-coated glass. The greater the cantilever's contact time with the surface, the more force and energy was required to retract from the surface. *E. coli*-coated cantilevers had more adhesion to *B. bacteriovorus* biofilms than to *E. coli* biofilms, but even *E. coli - B. bacteriovorus* interaction paled in comparison to adhesion between *E. coli* biofilms and abiotic surfaces. Further results probing biofilms with cantilevers that have been chemically modified with acid or amine groups will be presented.

3192-Pos Board B622
A Self-Consistent Multiscale Methodology for Predicting Adhesion of Mammalian Cells onto Functionalized Surfaces
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Predicting cell adhesion onto surfaces functionalized with peptides is inherently a multiscale problem since the adhesion interface is mediated largely by interactions of specific peptides with surface receptors. This interaction occurs over length scales on the order of nanometers, while typical mammalian cells are on the order of microns. In this work, we showcase a self-consistent approach for obtaining specifics of interactions between peptide sequences and receptors, and then applying this chemical information to describe these interactions for cells that are decorated with these receptors. Using this approach we present adhesion equilibrium behavior for 3 different receptor-peptide sequences across a range of length scales, from 50 nm, to 500 nm. We believe this approach offers a clear path to scaling up to mammalian cells (5-20 microns).

3193-Pos Board B623
Mapping Interactions between Silver Nanoparticles and Biomolecules at the Atomic Level
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The association of biomolecules with silver nanoparticles (AgNPs) has been shown to modify the nanoparticles' stability as well as their behavior in the physiological environment. However, the details of how silver nanoparticle surfaces – replete with heterogeneities – interact with the equally heterogeneous surfaces of biomolecules remain elusive, yet essential to understanding the origin of the biological activity of AgNPs. Leveraging molecular dynamics simulation and free-energy/kinetics calculations, we have constructed maps detailing interactions of bare and functionalized AgNPs with peptides, proteins, and lipid bilayer membranes.

3194-Pos Board B624
Protein Corona and Secondary Structure in Response to Nanoparticle Pegylation
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Nanoparticles are versatile tools for biophysical applications. Using these particles requires a close examination of the protein corona: the layer of proteins that adsorbs onto the particle surface. Modifying nanoparticle surfaces with polyethylene glycol (PEG) has been shown to reduce corona formation. Because tightly bound 'hard' corona proteins can block surface ligands that could be used in targeting applications, a reduction in corona is desirable and can enhance our ability to effectively utilize nanoparticle surface modifications. First, gold nanoparticles were PEGylated and characterized with dynamic light scattering. Using gel electrophoresis, a three-fold decrease in corona formation was found for PEGylated nanoparticles compared to bare nanoparticles. With a reduction of corona confirmed, we next investigated the secondary structure of the corona proteins. PEGylated and bare nanoparticles were incubated with bovine serum albumin, the most prevalent serum protein. Using CD spectroscopy, we probed the secondary structure of the adsorbed albumin. Significant structural changes were not detected. In addition, bovine serum albumin, α2-macroglobulin, and transferrin were each incubated with free PEG. Once again, no alteration of protein secondary structures were found, even in the presence of a one hundred molar excess of free PEG. These results conclude that PEG can quantitatively reduce corona formation without altering structural aspects of corona proteins.

3195-Pos Board B625
A Theoretical Study of Polymer-Based Drug Delivery Systems
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A variety of interactions between drug delivery devices and local cells and tissues impact clinical outcomes in terms of both therapeutic action and biological response. Understanding the competition of interactions in highly inhomogeneous environments such as those relevant in tissue engineering, nanotechnology, and those responsible for biological cell function is critical to the further development of design platforms for delivery systems. We use a three dimensional mean-field theory to study the competition between electrostatic, van der Waals and steric interactions in determining the molecular organization of micelles made of ampliphilic diblock polybases designed to carry doxorubicin to cancer cells. The micelles are assumed to target cancer cells primarily through electrostatic binding as several cancers are known to flip negatively charged lipids to the outer-leaflet. The polyelectrolyte micelles spontaneously form self-assembled aggregates whose physical properties are manipulated by the composition of the solution in contact with the polymer system. These theoretical calculations show that chemical equilibrium and the relevant physical interactions present in responsive polymer micelless couple in such

a highly non-additive manner that the qualitative physics can only be accurately determined through a highly detailed molecular theory.
We find that charge regulation stabilizes micellar domains over a wide range of pH by reducing the local charge in the aggregate at the cost of chemical free energy and gaining in the van der Waals attractive interactions. The balance of interactions in this highly inhomogeneous environment determines the boundaries between different carrier and release morphologies. We predict the formation of polymer micelle phases based on the proper choice of solution pH and salt concentration, and one can use these predictions to provide design guidelines for the creation of responsive polymer delivery systems presenting self-organized patterns with the desired functional properties.

3196-Pos Board B626
Red Blood Cell Behavior within the Exclusion Zone
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Various hydrophilic polymers have been reported to induce the formation of an exclusion zone (EZ) at their surface, which is devoid of particles and may extend to several hundred microns. It has previously been suggested that even cells may be excluded from the vicinity of the gel, thus raising the possibility of developing microscale cell-separation technologies. Here we explored the behavior of red blood cells (RBCs) in the vicinity of Nafion with the aim of devising a cell-separation method and of understanding the microscale mechanisms of EZ formation. We assembled a PDMS-based microfluidic device housing a 1-mm diameter, 50-micron thick cylinder of Nafion. A suspension of RBCs, prepared from anti-coagulated whole human blood by repeated washing/resuspension in PBS, was infused in the device. The position, shape and spectral properties of RBCs were followed with brightfield video microscopy. Contrary to expectations, RBCs were not excluded from Nafion surface. Rather, a three-phase process of aggregation, lysis and discoloration propagated gradually across the stationary RBC suspension from the Nafion surface towards distal regions. During the discoloration phase RBCs turned brown, pointing at the possibility of acid-hematin formation. Microscpectroscopy measurements supported this hypothesis. Thus, the vicinity of fresh Nafion surface is a highly acidic environment. The spatial and temporal propagation of the process suggests that protons diffuse out of the polymer. Soaking Nafion extensively in PBS resulted in the disappearance of the RBC-associated phenomenon, indicating that the thermodynamic driving force of particle exclusion is most likely the presence of a steep proton gradient between Nafion and the surrounding buffer solution. Due to its high acidity, unequilibrated Nafion has limited applications in cell-separation methodologies.

3197-Pos Board B627
Solid-Binding Peptides as a Biotemplate for Li-Ion Battery Electrodes
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Li-ion battery electrodes composed of electroactive materials at the nanoscale level show higher capacity and energy density over macroscale structures. However, nanoscale battery materials are prone to aggregation upon cell cycling, which reduces the specific capacity and coulombic efficiency, thus, leading to poor cycling stability. Using a biotemplating approach for electrode fabrication presents opportunities that may overcome aggregation and improve conductivity through introduction of biological nanoscale templates that would precisely control the position of electroactive nanoparticles in intimate proximity with conductive material and provide structural support upon cycling. Engineering of nanoscale bridges between electroactive and conductive material is done using solid-binding peptides (SBP) that have specific binding affinity for the materials of interest. In our study, SBP for cathode material Li2Mn3NiO8 (LMNO) was isolated using M13 bacteriophage through Phage Display procedure (New England Biolabs®). The nature of binding affinity between the peptide and the active material was determined through site-directed mutagenesis of specific amino acids in the peptide sequence. Binding peptides for LMNO and multiwalled carbon nanotubes (MWCNTs) are combined to form bifunctional peptide that serve as a nanobridge to connect two materials with synergistic properties. In this presentation I will discuss research on determining how SBPs bind to electroactive materials, and I will also show the impact that multifunctional SBPs have on improving battery electrode performance.

3198-Pos Board B628
Current Fluctuation Analysis in a Protein Nanopore
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Current fluctuation analysis has been widely used over the recent years to study the kinetic effects of different biological systems like neuronal networks or biomembranes. In particular, noise analysis has been successfully employed in protein ion channels to investigate the transport mechanisms that control the channel function. In this work, current fluctuations are analyzed in a protein nanopore, OmpF from E. coli. The study is performed for different electrolytes, including KCl, LiCl, $MgCl_2$, and $CaCl_2$, over a wide range of concentrations and voltages. Previous studies addressing current fluctuations in OmpF investigated the pH titration of the channel residues by analyzing the Lorentzian-like shape of the power spectral densities [1]. A complementary approach is followed here, based on the noise studies of Hoogerheide and colleagues in synthetic nanopores [2]. Special attention is paid to the additional white noise seen in the low frequency range of the power spectral density. The average noise scales with the square of the dc current, showing that this frequency−independent excess noise originates from conductance fluctuations. These fluctuations are analyzed here in terms of the ionic concentration to disclose the different transport mechanisms occurring in OmpF channel.
[1] E.M. Nestorovich et al. (2003) Biophys. J. 85:3718−3729
[2] D.P. Hoogerheide et al. (2009) Phys. Rev. Lett. 102:256804

3199-Pos Board B629
Naturally Synthetic: Using Biology to Improve Technology
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Nature has a diverse toolkit that can be utilized to address a broad array of problems. Among these tools are DNA, lipids, polysaccharides, and proteins, each of which has been used for direct applications from sensors to electronics. Among these macromolecules, proteins represent nature's most diverse polymer with a range of functionality determined by 20 different natural building blocks. The functionality of proteins is determined by their amino-acid content and structure. For instance proteins that bind to metal ions for biomineralization typically express higher levels of amino acid residues containing carboxylate side groups or histidines and cysteines. The amino acid makeup of a protein or polypeptide determines its properties (whether it can bind to metal ions, protein surfaces or nearly any other functional material because proteins can be designed to bind to a large number of materials).
The focus of my group is to identify functional polypeptides and use these to improve the properties of technologically relevant materials. Our lab uses a technique called phage display in order to identify solid binding polypeptides that are specific for binding to and the mineralization of electroactive materials and use these materials to prepare new lithium ion batteries. Once peptides are identified, they will be synthesized and combined with other peptide chains that have already been isolated that bind to carbon nanotubes (CNTs) to make multifunctional polypeptides. My research is multidisciplinary and involves the integration of biology, biochemistry, synthesis and nanomaterials science in order to address significant technological problems.